Russian Journal of Organic Chemistry 2011 vol.47 N1, pages 100-108

Experimental and theoretical study on 6-substituted pyridoxine derivatives. Synthesis of Cyclic 2,4,5,6-Tetrakis-(hydroxymethyl)pyridin-3-ol Acetonides

Shtyrlin N., Dobrynin A., Madzhidov T., Pugachev M., Sysoeva L., Musin R., Litvinov I., Klimovitskii E., Shtyrlin Y.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© Pleiades Publishing, Ltd., 2011. Synthetic approaches to three cyclic 2,4,5,6-tetrakis(hydroxymethyl)pyridin-3-ol acetonides were developed. Among seven possible mono- and diketals, six-membered cyclic ketal incorporating the hydroxymethyl group in the 4-position turned out to be the most thermodynamically favorable. The experimental data were consistent with the results of quantum-chemical calculations of the Gibbs energies of formation of different acetonides. The structure of the isolated compounds was studied by X-ray diffraction.

http://dx.doi.org/10.1134/S107042801101012X